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NRLMOL**

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I request a copy of the all-electron gaussian-orbital based Naval Research Laboratory Molecular Orbital Library (NRLMOL) for clusters and molecules.

**DEFINITIONS**

In the following, the term “the authors”, refers to M.R. Pederson, D.V. Porezag, J.Kortus, K.A. Jackson and D.C. Patton. ‘Program’ shall mean that copyrighted gaussian-orbital electronic structure code (in source, object and executable form) comprising the computer programs known as NRLMOL.

**MANDATORY TERMS AND CONDITIONS**

I will adhere to the following conditions upon receipt of the program:

1. All title, ownership and rights to NRLMOL or to copies of it remain with Mark R. Pederson, irrespective of the ownership of the media on which the program resides.
2. I will not supply a copy of NRLMOL to anyone for any reason whatsoever. This in no way limits my making copies of the code for backup purposes, or for running on more than one computer system at my institution. I will refer any request for copies of the program to the authors.
3. Without prior written consent of the authors, I will not incorporate any part of NRLMOL into any other computer code or program system.
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5. I understand that the authors supply NRLMOL and any documentation on an “as is” basis without any warranty, and thus with no additional responsibility or liability. I agree to report any difficulties encountered in the use of NRLMOL to the authors.
6. In any publication in the scientific literature I will make reference to:
  - M.R. Pederson and K.A. Jackson, Phys. Rev. B **41**, 7453 (1990).

- K.A. Jackson and M.R. Pederson, Phys. Rev. B **42**, 3276 (1990).
- M.R. Pederson, D.V. Porezag, J. Kortus and D.C. Patton, phys. stat. sol. (b) **217**, 197-218 (2000)

and, when appropriate, to one or more of the publications that appear in the copyright statement at the beginning of each run.

7. One copy of each and every publication resulting from use of NRLMOL will be filed in timely fashion with the first author, Mark R. Pederson.
8. It is understood that modifications of NRLMOL codes can lead to problems where the authors may not be able to help.
9. I understand that support for running the program can not be provided in general, except on the basis of a joint project between the authors and the research partner.
10. I will report useful modifications to the authors.

### Statement

I have read the above ten (10) terms and conditions and agree to abide by all of them.

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